

The Hellberg-Mele Jastrow factor as a variational wave function for the one dimensional XXZ model

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We find the Jastrow factor introduced by Hellberg and Mele in their study of the one dimensional $t - J$ model provides an exceedingly good variational description of the one dimensional XXZ model.

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The one dimensional systems are genuinely strongly correlated. This is most clearly indicated by the power law behavior of various correlation functions, which are termed Luttinger liquid behavior in general[1]. In a Luttinger liquid system, the powers of the correlation functions, or, the critical exponents of the system, are continuous functions of the model parameter.

The one dimensional XXZ model is typical Luttinger liquid system. In this short note, we propose a variational description this well known model. The Hamiltonian of the model reads

$$H = - \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z), \quad (1)$$

in which Δ is the parameter of anisotropy. This model is exact soluble in terms of the Bethe Ansatz[2]. For $\Delta < -1$, the system is in the Ising regime in which the ground state is antiferromagnetically ordered. For $\Delta > 1$, the system phase separates into full polarized regions. For $-1 < \Delta < 1$, which is the most interesting case, the system exhibits critical behavior with continuously varying critical exponents. For example, the asymptotic behavior of the transverse and the longitudinal spin correlation function are given by

$$\langle S_i^x S_j^x \rangle \sim \frac{A_x}{|i-j|^\eta} + (-1)^{i-j} \frac{\tilde{A}_x}{|i-j|^{\eta+1/\eta}} \quad (2)$$

and

$$\langle S_i^z S_j^z \rangle \sim \frac{A_z}{|i-j|^{1/\eta}} - (-1)^{i-j} \frac{1}{4\pi^2 \eta |i-j|^2}, \quad (3)$$

in which the critical exponent η is given by

$$\eta = \frac{1}{2} - \frac{1}{\pi} \sin^{-1} \Delta. \quad (4)$$

The last equation for the critical exponent η is obtained by combining the result of Bethe Ansatz solution and the effective field theory based on Abelian Bosonization[3]. Either the Bethe Ansatz solution or the effective field theory alone is not powerful enough to predict the critical

exponent. In the Bethe Ansatz approach, the wave function is so complicated that a direct calculation of the correlation function is impossible. On the other hand, while the essence of the critical correlation is well captured by the effective field theory approach, the parameters in the theory must be set by hand.

A good variational wave function should capture simultaneously the short range and the long range correlation of the system studied. However, for local Hamiltonian, it is difficult to get the correct long range behavior of the system by optimizing the energy of a variational wave function. Wave functions very close in energy can have drastically different long range behavior, provided that the system is in the critical regime.

We find a wave function originally proposed for the one dimensional $t - J$ model provides an excellent description of both the short range(energy) and the long range correlation of the one dimensional XXZ model for $-1 \leq \Delta \leq 1$. The wave function is given by

$$\Psi_{\text{HM}}(\{x_i\}) = \prod_{i < j} \sin\left(\frac{\pi(x_i - x_j)}{N}\right)^\nu, \quad (5)$$

in which x_i denotes the coordinates of the up spins in the periodic chain of N sites. This form is first proposed by Hellberg and Mele to describe the Luttinger liquid behavior of the one dimensional $t - J$ model[4]. In terms of the $t - J$ model, this function appears as a Jastrow factor for the residual charge correlation in front of the well known Gutzwiller projected Fermi sea wave function. For that purpose, one should reinterpret $\Psi_{\text{HM}}(\{x_i\})$ as a wave function for hard core Boson, in which x_i then denotes the coordinates of the charges(or holes) in the $t - J$ model.

The function introduced by Hellberg and Mele is also known as the exact ground state of the Sutherland model with inverse square interaction in one spatial dimension[5]. The Sutherland model reads,

$$H = - \sum_i \frac{\partial^2}{\partial x_i^2} + \frac{g\pi^2}{L^2} \sum_{i < j} \sin^{-2}\left(\frac{\pi(x_i - x_j)}{L}\right), \quad (6)$$

where the last term is a generalized inverse square potential on a periodic chain of length L . It is found that when

$$\nu = (\sqrt{2g+1} + 1)/2, \quad (7)$$

$\Psi_{\text{HM}}(\{x_i\})$ is the exact ground state of the Sutherland model.

In our recent work on the variational study of the one dimensional $t - J$ model, we find the residual charge correlation beyond the Gutzwiller projected wave function (GWF) of the model should be described by a XXZ-type effective Hamiltonian[6]. Combining this analysis and wave function proposed by Hellberg and Mele, one quickly realized that the Jastrow factor introduced by them should also be a good description of the ground state of the one dimensional XXZ model itself.

The reason for the excellentness of the Hellberg-Mele wave function for the one dimensional XXZ model can be more directly seen as follows. At $\Delta = 1$, the XXZ model reduces to that of the isotropic spin chain with ferromagnetic exchange, whose ground state is the fully polarized state. The wave function for the fully polarized state is a constant in the Ising basis, which is given exactly by $\Psi_{\text{HM}}(\{x_i\})$ with $\nu = 0$. At $\Delta = 0$, the model reduces to the one dimensional XX model, which is equivalent to the free spinless Fermion model through the Jordan-Wigner transformation. In this case, the ground state wave function is given exactly by $\Psi_{\text{HM}}(\{x_i\})$ with $\nu = 1$, a Slater determinant for the spinless Fermion. Another special case is when $\Delta = -1$. In this case, the model reduces to that of the isotropic spin chain with antiferromagnetic exchange. Although $\Psi_{\text{HM}}(\{x_i\})$ is no longer an exact ground state for this model, it is well known that the $\Psi_{\text{HM}}(\{x_i\})$ with $\nu = 2$, namely a Gutzwiller projected half filled Fermi sea wave function, provides a exceeding good variational description for the model considered[7]. For example, the energy calculated from $\Psi_{\text{HM}}(\{x_i\})$ is about -0.6921 per bond, which very close to the exact value, $-\ln 2$. At the same time, the long range correlation of the model is also correctly captured by this wave function, apart from a logarithmic correction which is absent for $\Delta > -1$.

The ground state energy and other ground state correlation of $\Psi_{\text{HM}}(\{x_i\})$ can be easily calculated by the Variational Monte Carlo method. Figure 1 shows the ground state energy calculated from $\Psi_{\text{HM}}(\{x_i\})$. We find the relative error in the ground state energy is less than 0.24 percent(which is reached at $\Delta = -1$) for all values of Δ .

The Hellberg-Mele-type wave function can not only give precise estimate for the ground state energy, but also give qualitatively correct behavior of the critical exponent of the model. In [8], it is found that the critical exponent η for $\Psi_{\text{HM}}(x_i)$ is simply given by $\frac{\nu}{2}$. In Figure 2, we compare the exact result for the critical exponent with that given by the Hellberg-Mele wave function. One find

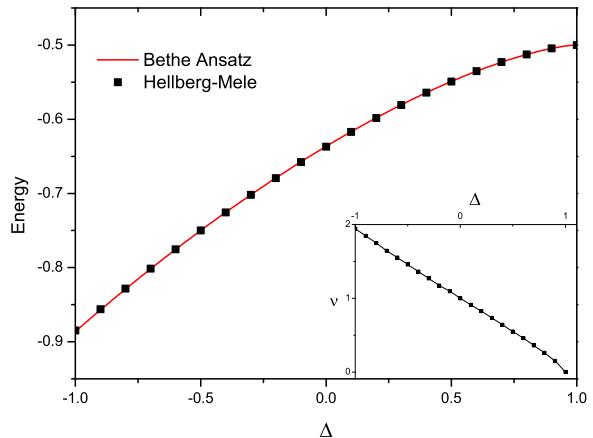


FIG. 1: Variational ground state energy calculated from $\Psi_{\text{HM}}(\{x_i\})$. The solid line shows the exact result obtained from Bethe Ansatz solution. The optimized value of the Δ is shown in the inset.

the variational result agree qualitatively with the exact one. Note for $\Delta = 1$, although the spin rotational symmetric GWF give the correct value of 1 for the critical exponent η , one find that in the variational description in terms of $\Psi_{\text{HM}}(x_i)$ the system chooses to break such symmetry slightly. We think this failure should be attributed to the logarithmic coorection at the symmetric point $\Delta = -1$.

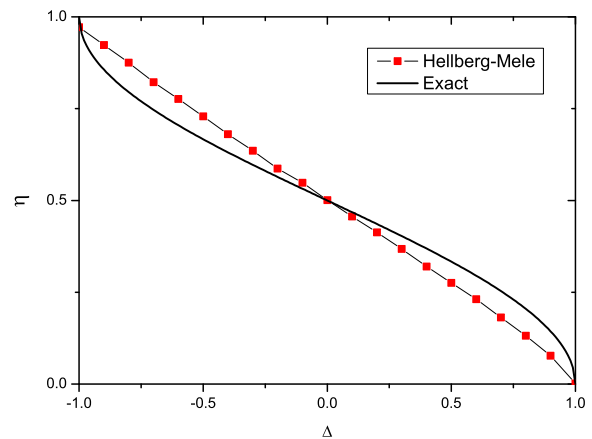


FIG. 2: Correlation exponent η as defined in Eq.(1) as determined from the Hellberg-Mele wave function. The solid line denotes the exact result $\eta = 1 - \frac{1}{\pi} \cos^{-1} \Delta$.

Finally, we note that although the Hellberg-Mele wave function is good approximation for the $S_{tot}^z = 0$ sector

of the one dimensional XXZ model, it fails to describe the physics of the $S_{tot}^z \neq 0$ sector of the same model. In [6], this is found to be responsible for the failure of the Hellberg-Mele-type wave function to describe the Luther-Emery phase at small electron density and large J/t of the one dimensional $t - J$ model.

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